

High-density correlation energy expansion of the one-dimensional uniform electron gas

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We show that the expression of the high-density (i.e small- r_s) correlation energy per electron for the one-dimensional uniform electron gas can be obtained by conventional perturbation theory and is of the form $\epsilon_c(r_s) = -\pi^2/360 + 0.00714 r_s + \dots$, where r_s is the average radius of an electron. Combining these new results with the low-density correlation energy expansion and the available diffusion Monte Carlo (DMC) data, we propose a local-density approximation correlation functional, which deviates by a maximum of 0.2 millihartree compared to the benchmark DMC calculations.

I. INTRODUCTION

While the high-density (small- r_s) reduced (i.e. per electron) correlation energy expansions

$$\begin{aligned}\epsilon_c(r_s) &= \sum_{j=0}^{\infty} (\lambda_j \ln r_s + \epsilon_j) r_s^j \\ &= \lambda_0 \ln r_s + \epsilon_0 + \lambda_1 r_s \ln r_s + \epsilon_1 r_s + \dots\end{aligned}\quad (1)$$

(where r_s is the Seitz radius) of the two-dimensional (2D) and three-dimensional (3D) uniform electron gas (UEG) are quite well-known,^{1–25} much less has been discovered about the one-dimensional (1D) UEG. This lack of information is mainly due to the divergence of the Coulomb operator $1/x$ in 1D for small interelectronic distance x ,^{26–30} which makes conventional perturbation theory difficult to apply due to the absence of Fourier transform for the Coulomb operator. Recently much attention has been devoted to such 1D systems, which can be experimentally realized in carbon nanotubes,^{31–35} organic conductors,^{36–40} transition metal oxides,⁴¹ edge states in quantum Hall liquids,^{42–44} semiconductor heterostructures,^{45–49} confined atomic gases,^{50–52} and atomic or semiconducting nanowires.^{53,54}

In this Article, we propose to fill this gap by reporting the values of the first few high-density coefficients (see Table I). The present system is constructed by allowing the number n of electrons in a 1D box of length L with periodic boundary conditions to approach infinity with the density $\rho = n/L$ held constant.^{55,56} Because the paramagnetic and ferromagnetic states are degenerate for strict 1D systems, we will consider only the latter.^{28–30}

To avoid the divergence of the Coulomb operator, we will consider in our derivation a “soften” version of the Coulomb operator $1/\sqrt{x^2 + R^2}$, where R is a parameter which removes the singularity at $x = 0$.^{57,58} Then, we will carefully take the limit $R \rightarrow 0$. We will show that, unlike the 2D and 3D version of the UEG, second- and third-order perturbation theories are convergent, i.e there is no need to use resummation techniques.¹³ Combining these new results with the low-density energy expansion and the available diffusion Monte Carlo (DMC) data, we propose a new local-density approximation (LDA) functional for the reduced correlation energy of the 1D UEG. Atomic units are used throughout.

II. HIGH-DENSITY EXPANSION

A. Second-order perturbation theory

In 1D, the spinorbitals of the free electron gas are

$$\psi_k(x) = \frac{e^{ikx}}{\sqrt{L}}, \quad (2)$$

with the energy $\kappa_k = k^2/2$, and where the periodic boundary conditions imply $k = 2\pi m/L$ ($m \in \mathbb{Z}$). The coefficient ϵ_0 is given by second-order perturbation theory⁵⁹

$$\epsilon_0(R) = \frac{1}{4n} \sum_{ab}^{\text{occ}} \sum_{rs}^{\text{virt}} \frac{|\langle ab||rs \rangle|^2}{\kappa_a + \kappa_b - \kappa_r - \kappa_s}, \quad (3)$$

where $\langle ab||rs \rangle = \langle ab|rs \rangle - \langle ab|sr \rangle$ and

$$\langle ab|rs \rangle = \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \frac{\psi_a^*(x_1) \psi_b^*(x_2) \psi_r(x_1) \psi_s(x_2)}{\sqrt{(x_1 - x_2)^2 + R^2}} dx_1 dx_2. \quad (4)$$

The constant coefficient ϵ_0 is usually decomposed in a direct (“ring-diagram”) term ϵ_0^a and an exchange term ϵ_0^b , which read explicitly

$$\epsilon_0^a(R) = \frac{1}{2n} \sum_{ab}^{\text{occ}} \sum_{rs}^{\text{virt}} \frac{\langle ab|rs \rangle \langle rs|ab \rangle}{\kappa_a + \kappa_b - \kappa_r - \kappa_s}, \quad (5)$$

$$\epsilon_0^b(R) = -\frac{1}{2n} \sum_{ab}^{\text{occ}} \sum_{rs}^{\text{virt}} \frac{\langle ab|rs \rangle \langle rs|ba \rangle}{\kappa_a + \kappa_b - \kappa_r - \kappa_s}. \quad (6)$$

TABLE I. High-density coefficients for the paramagnetic state of the 1D, 2D and 3D UEGs. The paramagnetic and ferromagnetic states are degenerate in 1D. β and ζ are the Dirichlet beta and Riemann zeta function, respectively.⁶⁰

Coefficient	Term	1D	2D	3D
λ_0	$\ln r_s$	0	0	$(1 - \ln 2)/\pi^2$
ϵ_0	r_s^0	$-\pi^2/360$	$\ln 2 - 1 + \beta(2) - 8\beta(4)/\pi^2$	$-0.071099 + (\ln 2)/6 - 3\zeta(3)/(4\pi^2)$
λ_1	$r_s \ln r_s$	0	$-\sqrt{2}(10/(3\pi) - 1)$	$+0.009229$
ϵ_1	r_s	$+0.00714$	unknown	-0.020

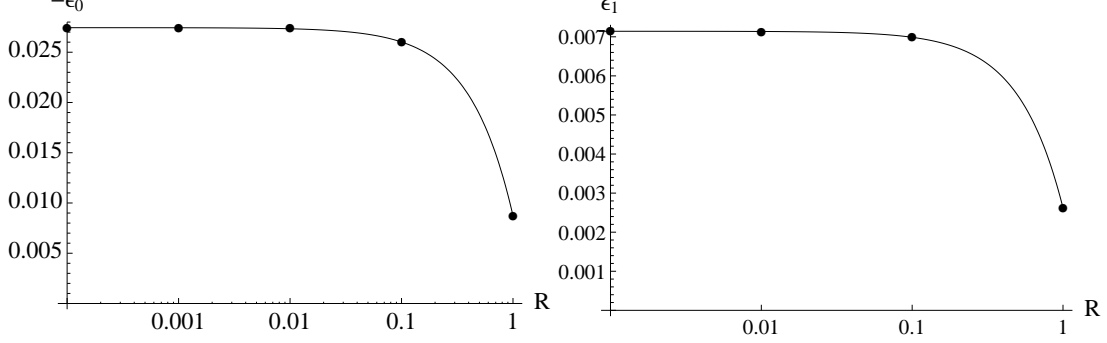


FIG. 1. Convergence of ϵ_0 and ϵ_1 with respect to R .

Using the Fourier transform of the soft Coulomb potential

$$\frac{1}{\sqrt{x^2 + R^2}} = \frac{1}{\pi} \int_{-\infty}^{\infty} K_0(|k|R) e^{ikx} dk, \quad (7)$$

where K_0 is the zeroth-order modified Bessel function of the second kind⁶⁰, the well-known relation

$$\delta(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} dk, \quad (8)$$

and transforming the sums in (5) and (6) into integrals with $p_1 = a/k_F$, $p_2 = b/k_F$ and $q = k/k_F$, where $k_F = \pi\rho$ is the Fermi wave vector, we eventually find⁶¹

$$\epsilon_0^a(R) = -\frac{1}{4\pi^2} \int_{-\infty}^{\infty} dq \int_{\substack{|p_1| < 1 \\ |p_1+q| > 1}} dp_1 \int_{\substack{|p_2| < 1 \\ |p_2+q| > 1}} dp_2 \frac{K_0(|q|R)^2}{q(p_1 + p_2 + q)}, \quad (9)$$

and

$$\epsilon_0^b(R) = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} dq \int_{\substack{|p_1| < 1 \\ |p_1+q| > 1}} dp_1 \int_{\substack{|p_2| < 1 \\ |p_2+q| > 1}} dp_2 \frac{K_0(|q|R)K_0(|p_1 + p_2 + q|R)}{q(p_1 + p_2 + q)}. \quad (10)$$

For $R > 0$, Eqs. (9) and (10) can be evaluated numerically. As shown in Fig. 1, $\epsilon_0(R)$ decreases monotonically to reach a constant at $R = 0$. However, for $R = 0$, both integral diverge with opposite rate. Thus, to find the limiting value, it is better not to split $\epsilon_0(R)$ into two contributions but to consider them together. For small R , we have

$$\epsilon_0(R) = -\frac{1}{2\pi^2} \int_0^{\infty} dq \int_{\substack{|p_1| < 1 \\ |p_1+q| > 1}} dp_1 \int_{\substack{|p_2| < 1 \\ |p_2+q| > 1}} dp_2 \frac{[\ln q - \ln(p_1 + p_2 + q)][\ln(qR/2) + \gamma]}{q(p_1 + p_2 + q)} + O(R^2). \quad (11)$$

The integrations over p_1 and p_2 can be performed at this stage and it yields

$$\epsilon_0(R) = -\frac{1}{4\pi^2} \int_0^{\infty} \frac{\Lambda(q)}{q} [\ln(qR/2) + \gamma] dq, \quad (12)$$

where γ is the Euler-Mascheroni constant⁶⁰ and

$$\begin{aligned}\Lambda(q) &= (2+q)[\ln(2+q)]^2 + (2-q)[\ln(2-q)]^2 \\ &\quad - 2(1+\ln q)(2+q)\ln(2+q) \\ &\quad - 2(1+\ln q)(2-q)\ln(2-q) \\ &\quad - 4(\ln 2)^2 + 8\ln 2(1+\ln q)\end{aligned}\tag{13}$$

for $0 \leq q \leq 2$, and

$$\begin{aligned}\Lambda(q) &= (2+q)[\ln(2+q)]^2 + (2-q)[\ln(q-2)]^2 \\ &\quad - 2(1+\ln q)(2+q)\ln(2+q) \\ &\quad - 2(1+\ln q)(2-q)\ln(q-2) \\ &\quad + 2(2+\ln q)q\ln q\end{aligned}\tag{14}$$

otherwise. Performing the last integration over the two distinct regions ($0 \leq q \leq 2$ and $q > 2$) gives two contributions which diverges as $\ln R$ for small R with opposite sign. Thus, the divergences cancel and we find

$$\epsilon_0 = \lim_{R \rightarrow 0} \epsilon_0(R) = -\frac{\pi^2}{360},\tag{15}$$

which nicely reproduces the result obtained with a ring geometry.³⁰

Because $\epsilon_c(r_s) = \epsilon_0 + O(r_s)$ (see below), ϵ_0 provides the *exact* value of the correlation energy at $r_s = 0$, and it is roughly -27.4 millihartree per electron. It is worth noting that, in most of the studies on 1D systems, a soft Coulomb operator is considered. For example, in Refs. 62 and 63, the authors used $R = 1$, yielding a correlation energy (-8.7 millihartree) more than three times lower than the value obtained using the genuine Coulomb operator (i.e $R = 0$). Moreover, using a quasi-1D model with a transverse harmonic potential, Casula et al. conclude that, in the high-density limit, the correlation energy vanishes quadratically with r_s .⁶⁴ This strikingly different prediction stresses the importance of employing a realistic Coulomb operator

B. Third-order perturbation theory

Using the same approach, third-order perturbation theory gives⁵⁹

$$\begin{aligned}\epsilon_1(R) &= \frac{1}{8n} \sum_{abcdrs} \frac{\langle ab||rs \rangle \langle cd||ab \rangle \langle rs||cd \rangle}{(\kappa_a + \kappa_b - \kappa_r - \kappa_s)(\kappa_c + \kappa_d - \kappa_r - \kappa_s)} \\ &\quad + \frac{1}{8n} \sum_{abrstu} \frac{\langle ab||rs \rangle \langle rs||tu \rangle \langle tu||ab \rangle}{(\kappa_a + \kappa_b - \kappa_r - \kappa_s)(\kappa_a + \kappa_b - \kappa_t - \kappa_u)} \\ &\quad + \frac{1}{n} \sum_{abcrst} \frac{\langle ab||rs \rangle \langle cs||tb \rangle \langle rt||ac \rangle}{(\kappa_a + \kappa_b - \kappa_r - \kappa_s)(\kappa_a + \kappa_c - \kappa_r - \kappa_t)}.\end{aligned}\tag{16}$$

Equation (16) can be decomposed, using the same transformations as in (9) and (10), into six distinct contributions:

$$\begin{aligned}\epsilon_1(R) &= -\frac{1}{\pi^4} \int dq d^3p \frac{v_R(q)^3}{q(p_1 + p_2 + q)q(p_1 + p_3 + q)} \\ &\quad + \frac{1}{\pi^4} \int dq d^3p \frac{v_R(q)^2 v_R(p_1 - p_2)}{q(p_1 + p_3 + q)q(p_2 + p_3 + q)} \\ &\quad + \frac{2}{\pi^4} \int dq d^3p \frac{v_R(q)^2 v_R(p_1 + p_2 + q)}{q(p_1 + p_2 + q)q(p_1 + p_3 + q)} \\ &\quad + \frac{2}{\pi^4} \int dq d^3p \frac{v_R(q) v_R(p_1 + p_2 + q) v_R(p_2 - p_3)}{q(p_1 + p_2 + q)q(p_1 + p_3 + q)} \\ &\quad + \frac{1}{\pi^4} \int d^2q d^2p \frac{v_R(q_1) v_R(q_2) [v_R(q_1 - q_2) - v_R(p_1 - p_2)]}{q_1(p_1 - p_2)q_2(p_1 - p_2)} \\ &\quad - \frac{1}{2\pi^4} \int d^2q d^2p \frac{v_R(q_1) v_R(q_2) [v_R(q_1 - q_2) - v_R(p_1 + p_2 + q_1 + q_2)]}{q_1(p_1 + p_2 + q_1)q_2(p_1 + p_2 + q_2)}\end{aligned}\tag{17}$$

TABLE II. Reduced correlation energy ($-\epsilon_c(r_s)$ in millihartree) for various r_s . The DMC and ISI results are taken from Refs. 28 and 30, respectively. Subscripts represent the statistical errors in the last digits. The deviation with respect to the DMC result is given in parenthesis.

r_s	DMC	ISI	This work
0	—	27.416	27.416
0.1	—	26.632	26.714
0.2	—	25.900	26.039
0.5	—	23.964	24.191
1.0	21.444 1 ₂	21.392 (−0.052)	21.648 (+0.204)
2.0	17.922 02 ₇	17.763 (−0.159)	17.990 (+0.068)
5.0	12.317 74 ₂	12.091 (−0.227)	12.226 (−0.092)
10.0	8.292 096 ₉	8.121 (−0.171)	8.196 (−0.096)
15.0	6.319 404 ₄	6.195 (−0.124)	6.246 (−0.073)
20.0	5.132 504 ₂	5.039 (−0.094)	5.077 (−0.056)

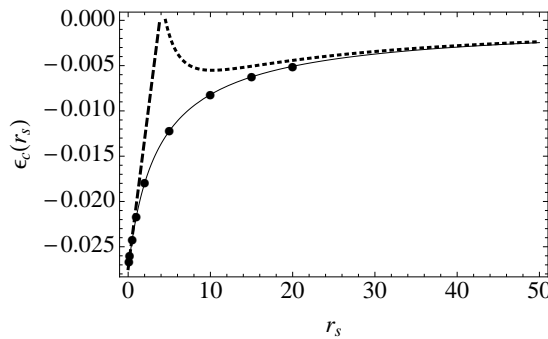


FIG. 2. $\epsilon_c(r_s)$ given by Eq. (21) as a function of r_s (solid line). DMC results are shown by black dots. The small- r_s expansion of Eq. (19) (dashed line) and large- r_s approximation of Eq. (20) (dotted line) are also shown.

where $v_R(q) = K_0(|q|R)$ and $\int d^m p = \int \dots \int dp_1 \dots dp_m$. The regions of integration are $|p_i| < 1$ and $|p_i + q| > 1$ for the first four integrals, and the fifth integral is over the region: $|p_1 + q_1| > 1$, $|p_1 + q_2| > 1$, $|p_1| < 1$; $|p_2 + q_1| < 1$, $|p_2 + q_2| < 1$, $|p_2| > 1$. The final integral is the sum of two parts, one over the region $|p_1 + q_1| > 1$, $|p_1 + q_2| > 1$, $|p_1| < 1$; $|p_2 + q_1| > 1$, $|p_2 + q_2| > 1$, $|p_2| < 1$; the second over the region the opposite inequalities.

Again, for $R = 0$, most of the integrals diverge. The first five terms have to be considered together, while the two parts of the last integral are finite. Evaluating numerically each of the contributions and extrapolating the result to $R = 0$ using the relation $\alpha R^\beta + \epsilon_1$ (see Fig. 1), we find

$$\epsilon_1 = \lim_{R \rightarrow 0} \epsilon_1(R) = 0.00714(1), \quad (18)$$

where the error has been obtained by taking into account each numerical error estimate and extrapolating the overall error to $R = 0$.⁶⁵ We note that the present 1D UEG is one of the few systems where the r_s coefficient of the high-density expansion is known.^{20,22} Moreover, the “line” geometry considered here seems to be more mathematically convenient (at least numerically) for deriving the r_s coefficient than the ring geometry of Ref. 30.

In summary, we have shown that the high-density correlation energy expansion (1) of the 1D UEG is

$$\epsilon_c(r_s) = -\frac{\pi^2}{360} + 0.00714 r_s + \dots \quad (19)$$

We note that, contrary to the 2D and 3D UEGs, the expansion (19) does not contain any logarithm term up to first order in r_s , i.e. $\lambda_0 = \lambda_1 = 0$ (cf Eq. (1)).

III. LDA FUNCTIONAL

It is known^{30,58} that the low-density (large- r_s) expansion of the correlation energy is

$$\begin{aligned}\epsilon_c(r_s) &= \frac{\eta_0}{r_s} + \frac{\eta_1}{r_s^{3/2}} + \dots \\ &= -\frac{\ln(\sqrt{2\pi}) - 3/4}{r_s} + \frac{0.359933}{r_s^{3/2}} + \dots\end{aligned}\quad (20)$$

Using the “robust” interpolation proposed by Cioslowski⁶⁶ and the high- and low-density expansions (19) and (20), the correlation energy can be approximated by

$$\epsilon_c(r_s) = t^2 \sum_{j=0}^3 c_j t^j (1-t)^{3-j}, \quad (21)$$

with

$$t = \frac{\sqrt{1 + 4k r_s} - 1}{2k r_s}, \quad (22)$$

and

$$c_0 = k \eta_0, \quad c_1 = 4k \eta_0 + k^{3/2} \eta_1, \quad (23)$$

$$c_2 = 5 \epsilon_0 + \epsilon_1/k, \quad c_3 = \epsilon_1, \quad (24)$$

where $k = 0.3083$ is a scaling factor which is determined by a least-square fit of the DMC data given in Ref. 28.

We disagree with the last comment made in Ref. 66, which claims that this type of interpolation is not applicable to cases where the high- and low-density asymptotic expansions pertain to *de facto* different states, e.g. the 3D UEG. We claim that the non-applicability of such a interpolation is only due to the presence of logarithmic terms in the 2D and 3D UEGs. However, in our case, the 1D UEG does not involve any non-analytical term. Thus, the methodology of Ref. 66 is obviously applicable in the present case.

The results using the new correlation functional (21) are compared to the DMC calculations of Lee and Drummond²⁸ and to our recently proposed correlation functional based on a ring geometry³⁰ and the “interaction-strength interpolation” (ISI) formula proposed by Seidl and co-workers.^{67,68} The results are gathered in Table II and depicted in Fig. 2. As one can see, our new correlation functional reduces the error of the ISI functional by a factor two (expect for $r_s = 1$ where the ISI functional is in better agreement with the DMC value). This overall improvement is expected because our new functional (21) contains one more information on the high-density limit than the correlation functional reported in Ref. 30.

IV. CONCLUSION

In this Article, we have shown that the expression of the high-density correlation energy for the 1D UEG is $\epsilon_c(r_s) = -0.02742 + 0.00714r_s + \dots$. Combining these new results with the low-density correlation energy expansion $\epsilon_c(r_s) = -[\ln(\sqrt{2\pi}) - 3/4] r_s^{-1} + 0.359933 r_s^{-3/2} + \dots$ and the available diffusion Monte Carlo data, we have proposed a LDA correlation functional, which yields satisfactory estimates of the correlation energy at high, intermediate and low densities.

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